Spectroscopic Study on Novel Photoactive Antibacterial Agent: 2, 3 – Distyrylindole.

Ruwini D. Rajapaksha and Mahinda I. Ranasinghe*

Department of Chemistry, New Mexico Institute of Mining and Technology, Socorro, NM87801

Key words: Multiphoton absorption, Photodynamic inactivation, Fluorescence decay kinetics.

Abstract:

Optical properties of novel, photoactive, indole based antibacterial chromophore system of, 2, 3 – distyrylindole (23DSI) molecule studied using various spectroscopic techniques as well as density functional theory (DFT) calculations. The spectroscopic techniques involved with UV-Vis spectroscopy, Fluorescence spectroscopy, Time-resolved fluorescence upconversion spectroscopy (TRFLS), and Time correlated single photon counting spectroscopy (TCSPC) were utilized. The studies show that the molecule 23DSI has multiphoton absorption showing two photon and three photon absorptions in both solid and solution phases. The multiphoton absorption characteristics of this molecule can be used in various applications such as fluorescence microscopy, 3-D optical storage, optical power limiting, photodynamic therapy (PDT), and photodynamic inactivation (PDI). The TRFLS studies on 23DSI molecule shows fast, single exponential decay with average time constant of 34 ps with average lifetime of 1ns. The NIR emission studies did not show any sign of singlet oxygen production of this molecule. The DFT calculations show that the 23DSI molecule has conjugated electron densities, which is responsible for multiphoton absorption. Both optical spectrum and emission wavelength using DFT calculations show excellent agreement with experimentally measured UV-Vis spectrum and emission wavelength. Combined experimental and theoretical studies suggest that relaxation of excited state electron to the singlet state (S_1) by internal conversion (IC) first and latterly relax back to their ground state (S_0) by emitting fluorescence. Due to the fast depopulation of S_1 to S_0 via fluorescence emission, there is no effective energy transferring occurs to the triplet state (T_1) of molecule and hence no successful singlet oxygen production.

*Corresponding author: mahinda.ranasinghe@nmt.edu